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6. AUTHOR(S) Ke Liu Marina Pantazidou	

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13. ABSTRACT (Maximum 200 words)

This research investigated how numerical modeling of dense nonaqueous liquid phase (DNAPL) spills can assist in the planning of field experiments of controlled DNAPL releases. The procedure was first validated using existing data from a controlled release at the Borden test site, and then extended to hypothetical releases at the Dover site. The simulation results confirmed that the total release volume, the infiltration rate and the DNAPL injection head are important parameters for the design of controlled release experiments. Specifically, it was found that proper selection of the injection head and the release volume through several numerical simulations can aid in controlling the extent of the DNAPL-contaminated area in the field. Finally, it was shown that considerable savings in computational time can be achieved by approximating the 3-D geometry with radial symmetric 2-D simulations. This is true provided that the soil distribution is relatively homogeneous at the horizontal plane, as it is the case at both Borden and Dover.

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NUMERICAL MODELING OF EXPERIMENTAL DNAPL RELEASE AT DOVER AFB

by
Ke Liu
and
Marina Pantazidou

1. Introduction

Field experiments are being planned and conducted at the Air Force Groundwater Remediation Field Laboratory (GRFL), Dover Air Force Base, Delaware, to demonstrate innovative site characterization, monitoring, and treatment techniques for remediation of NAPL-contaminated sites. A controlled release of tetrachloroethylene (PCE), a commonly detected dense nonaqueous phase liquid (DNAPL), into a saturated, 10x10 m test cell was planned to take place at this site. The work presented herein is aimed at providing assistance during the design phase of such controlled release experiments.

This project comprises three phases. The first phase involved the review of existing relevant experimental and numerical modeling studies to identify the important design parameters for a controlled DNAPL release in the saturated zone. The second phase involved reviewing site characterization data for the Dover site, evaluating the usefulness of these data for providing input parameters for multiphase flow numerical codes, and giving recommendations on improving site characterization for more accurate modeling of release experiments and for creating a complete data set for code validation. The third phase involved numerical simulations of past controlled releases conducted at the Canadian Forces base at Borden, Ontario, and hypothetical releases at the Dover site. The Borden site simulations were conducted partly for calibration purposes. Specific objectives of these simulations included: (i) testing the feasibility of modeling only large-scale subsurface features (such as major impermeable layers) to predict the main features of DNAPL distribution (such as DNAPL pools), and (ii) investigating the effect of source conditions on the relationship between computed flux and specified constant head at the DNAPL source. The objectives of the Dover site simulations were to investigate the effect of design parameters, such as the injection head, on DNAPL migration, and to help establish a decision-making strategy for specifying release conditions. The Dover site simulations considered both radially symmetric (2-D) and three-dimensional (3-D) domains to evaluate the ability of the 2-D simulations to capture the major features of the 3-D simulations. Thus the project included the following components: a literature review, a review of subsurface characterization data at the Dover site, and numerical simulations of releases at the Borden and Dover sites. These components are described in Sections 2-4 of this report, followed by a summary of the significant findings and recommendations in Section 5.

2. Literature review

Two controlled releases of PCE into a saturated aquifer at the Canadian Base at Borden (Kueper et al., 1993; Brewster et al., 1995) were reviewed. The horizontal dimensions of the cells were 3x3 m and 9x9 m. Both cells reached a depth of 3.4 m. The PCE head at the source was 1.23 m (corresponding to 1.98 m of water) for both releases. Although the two cells are only 10 m apart, and the aquifer is relatively homogeneous, the measured infiltration rates differed by as much as 38%, indicating that the infiltration rate is highly sensitive to minor changes in soil properties. The distributions of residual PCE were also quite different in the two cells. Significant lateral spreading of PCE along numerous, small-scale laminations was observed in the 3x3 m cell, whereas in the 9x9 m cell most of the PCE was contained in discrete pools located on top of low-permeability layers. The data from these two experiments suggest that for a sandy aquifer, a ratio of PCE injection volume to total pore volume on the order of magnitude of 10^{-3} - 10^{-2} may result in sufficient distribution in a test cell in the scale of meters, under an injection head of 1 - 2 m H_2O.

Numerical modeling prior to an experimental release can aid in understanding the relationship between the injection volume, the injection head, and the shapes of PCE distribution, and in controlling extensive lateral spreading. Existing numerical simulations for multiphase flow in hypothetical stochastic fields have provided valuable insights on those relationships (Essaid and Hess, 1993; Kueper and Gerhard, 1995). Most importantly, these simulations showed that different soil structures result in different relationships between the injection head and lateral spreading, indicating that the effect of boundary conditions on the DNAPL distribution has to be studied for specific soil structures. The numerical simulations of the present study were designed to further explore these relationships for soil conditions similar to those at the Borden and Dover sites.

3. Data review for Dover site

Existing site characterization data [GRFL CD-ROM (1995); GRFL Report (1996),] were reviewed to obtain the necessary input data for numerical modeling. Site characterization methods used at the Dover site include: (i) surface geophysical surveys on a 10x10 m grid covering a 60x140 m area; (ii) cone penetration test (CPT) borings at 59 locations; (iii) grain size analysis for soil samples from various depths at eight

locations; (iv) two pumping tests and a number of slug tests to determine the hydraulic conductivity of the aquifer; (v) CPT dissipation tests to estimate the hydraulic conductivity for the aquitard; and (vi) an instantaneous profile (IP) unsteady drainage flux test in the vadose zone to determine the conductivity of the unsaturated zone and the capillary pressure-saturation curve.

In general, a numerical simulation of a multiphase flow problem requires the following input parameters: fluid properties such as density and viscosity, spatially variable soil properties including permeability and porosity, and the constitutive relationships for the soil-fluid system, i.e., the capillary pressure-saturation and relative permeability-saturation relationships. As much as the available characterization data for the Dover site constitute a comprehensive hydrogeologic data set, they are limited in terms of providing input parameters for a numerical code of multiphase fluid flow. More specifically, the large-scale measurements on hydraulic conductivity (K) cannot be used to estimate the spatial variation of K within the test cell. Furthermore, the estimated constitutive relationships on the basis of grain size distribution data differed significantly from measurements. As a result, the grain-size distribution data are of little use for the prediction of constitutive relationships. Additionally, the constitutive relationships measured from the vadose zone IP test are average values over 3×3 m horizontal layers and hence are directly applicable only for homogeneous cross sections. Finally, the porosity variation in the vadose zone is not available. Only the CPT data provide fine-scale vertical variations of the soil classification number (SCN), from which hydraulic conductivity can be estimated within one order of magnitude accuracy. These CPT data were used herein to provide a 3-D estimation of SCN and K for the entire site through kriging.

The following procedures are recommended to improve the estimation of soil properties in a test cell: conducting CPT tests at locations closer to the test cell, conducting high resolution geophysical surveys for the test cell, conducting laboratory measurements of constitutive relationships, and establishing more accurate correlations between soil properties and soil type.

4. Numerical modeling

In this study, numerical simulations were performed using the T2VOC module of the TOUGH family of codes, which was developed at Lawrence Berkeley Laboratory (Falta

et al., 1995). The T2VOC simulator can model three-phase, three-component, non-isothermal flow of water, air and a volatile organic compound (VOC) in three-dimensional heterogeneous porous media. It requires the following soil-specific input parameters: permeability, porosity and the capillary pressure-saturation and relative permeability-saturation curves.

Eight numerical simulations were conducted for the 9x9 m cell test at the Borden site, considering a 2-D flow domain (i.e., assuming radial symmetry). One 3-D and four 2-D simulations were conducted for hypothetical releases at the Dover site.

In the Borden site simulations, a single low-permeability layer was modeled in an otherwise homogeneous test cell, using hydraulic conductivity (K) values published in the literature. For the Dover site, a geostatistical analysis (variogram calculation) was performed using the existing soil classification number (SCN) data. Based on the variogram, ordinary kriging calculations were used to predict the SCN distribution in the test cell. The input parameters required by T2VOC were obtained through the correlation between K and SCN, and the scaling relationship between the capillary pressure and K.

The Borden site simulations were successful in reproducing the largest of the experimentally observed PCE pools that were formed above low-permeability layers. In constant-head simulations, different combinations of PCE pressure and saturation specified for the source soil all resulted in identical infiltration rates and shapes of the PCE pool similar to that observed in the experiment. It is therefore recommended to measure the DNAPL saturation at the source during a controlled release, both for better understanding of the physical phenomena and for more accurate numerical modeling results. Additional sensitivity analyses showed that the specified mobility of water in the source elements and the weighting schemes at element interfaces do not have a big influence on modeling results, for the release conditions considered herein. On the contrary, modifying soil properties close to the PCE source confirmed that the infiltration rate is sensitive to near-source soil conditions.

For the Dover site, three 2-D simulations with different PCE injection heads were conducted. The results indicate that for the same release volume, a higher injection head results in a smaller total contaminated area, a shorter front, a wider spreading of PCE near the source, and a smaller width of maximum PCE spreading. The simulations also showed that the uncertainty in soil property estimation influences the predicted

infiltration rate more than the considered variations in the injection head (1.3 to 2.1 m).
During a controlled release with constant-head injection therefore, it is prudent to
monitor the infiltration rate and, if necessary, control the total injection volume, instead
of depending on an accurate prior prediction of the infiltration rate. Under the same
boundary conditions, 3-D and 2-D simulations resulted in less than 50% difference in
infiltration rates and similar shapes of PCE pools. Hence it was concluded that for soil
variability comparable to that at the Dover site, 2-D radial symmetric simulations are
accurate enough to capture the main features of DNAPL migration.

5. Significant Findings and Recommendations

♦ Review of existing field experiments and modeling studies confirmed that the total
release volume, the infiltration rate and the DNAPL injection head are important
parameters for the design of controlled release experiments.

♦ Among site characterization data commonly collected at a site, large-scale
measurements of hydraulic conductivity and soil grain size distribution are of little
use as input information for numerical modeling of NAPL transport. Kriging on soil
classification numbers determined from CPT tests can lead to estimation of the
required input soil properties.

♦ Numerical simulations for a reported field experiment indicate that water saturation at
the DNAPL source might be much higher than irreducible water saturation;
monitoring the source saturation during the infiltration stage is recommended.

♦ Selection of the injection head and the release volume through numerical simulations
is a good strategy to control the extent of the total DNAPL-contaminated area.
However, uncertainties in the soil property estimates result in significant uncertainty
in the predicted rate of DNAPL infiltration. Monitoring the infiltration rate and
controlling the total injection volume in the field are preferable than relying on an
accurate prior estimate of the infiltration rate.

♦ Radial symmetric 2-D simulations yield good approximations of the infiltration rates
and shapes of the DNAPL-contaminated area predicted by 3-D simulations, provided
that the soil type distribution is relatively homogeneous at the horizontal plane.

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NUMERICAL MODELING OF EXPERIMENTAL DNAPL RELEASE
AT DOVER AFB

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Ke Liu and Marina Pantazidou
Department of Civil and Environmental Engineering
Carnegie Mellon University

Abstract

The task of determining the extent of contamination at dense nonaqueous phase liquid (DNAPL) sites is a difficult one, because of the complexity of DNAPL distribution in the subsurface and the limitations of field characterization techniques. Conventional characterization methods, such as Shelby-tube soil samples and monitoring wells, are expensive and ineffective in providing the spatial details required for DNAPL transport studies. Recent studies on geophysical methods, including ground penetrating radar, neutron probe, time domain reflectometry, have yielded promising results for monitoring DNAPL transport over time (in the saturated zone). Complementing field characterization efforts, numerical modeling may provide insightful estimates of the DNAPL distribution in cases of known release histories. However, current immiscible flow numerical codes have undergone very limited verification against field experimental data. Field experiments of controlled DNAPL releases are necessary for evaluating the performance of both geophysical methods and numerical codes. A controlled release of a commonly detected DNAPL, tetrachloroethylene (PCE), was planned to take place within an isolated test cell at Dover Air Force Base. The high cost and complexity of such field experiments call for careful planning. Numerical simulations can provide valuable assistance during the design phase of these experiments.

The purpose of combining experimental and numerical modeling can, hence, be twofold: to assist in the planning of the experimental release and to establish the extent at which multiphase flow codes can serve as predictive tools. In this study, numerical simulations are performed using the T2VOC module of the TOUGH family of codes, which was developed at Lawrence Berkeley Laboratory. Prior to the modeling, existing field experiment and numerical modeling studies were reviewed to help identify the important design parameters of the DNAPL release. The available subsurface data provided by the test site manager at Dover Air Force Base were analyzed to determine the values of soil properties needed as input data for the numerical simulations. Considering uncertainty in site characterization, alternative scenarios of subsurface structures inside the cell are constructed for the simulations and referred to herein as different medium formations. By changing the infiltration head in the simulation for each formation, the range of the optimum release conditions can be established. Future work will include a study of the effects of uncertainty in input data parameters on the outcome quantities of interest, such as the vertical speed and horizontal spread of the DNAPL contaminant front.

1. Review of Existing Field Experiments/Modeling

To date, two controlled field releases of PCE in saturated soil have been conducted at the Borden site (Kueper et al., 1993; Brewster et al., 1995). The experimental conditions of the two releases were similar to those proposed for the PCE release at Dover Air Force Base. Similarities include the scale of the test cell, soil type, the DNAPL and the geophysical method used. Reviewing the data from the two experiments is helpful for the design of the planned controlled release. The important parameters are listed in Table 1. In both releases, the DNAPL infiltration took place under constant head conditions. The observed infiltration rates remained constant shortly after the initialization of the PCE release.

Table 1. Data from controlled PCE releases at Borden site.

	Field release 1 (Kueper et al.,1993)	Field release 2 (Brewster et al., 1995)
Test cell size	3m×3m×3.4m	9m×9m×3.4m
PCE volume	230.9 L	770 L
PCE volume/total pore volume	17.2	6.38
Release rate	8 L/Hr	11 L/Hr
Infiltration duration	28.9 Hr	70 Hr
Redistribution duration	28 days	41 days
Capillary pressure at source	16.6 kPa	15.1 kPa
Source diameter	14.92 cm	14.92 cm
Residual PCE saturation	$\leq 38\%$	$\leq 20\%$

Through two-dimensional (2-D) numerical simulations of hypothetical release cases, Kueper and Gerhard (1995) studied the influence of the location, size and DNAPL head of the contaminant source on the infiltration rate and lateral spreading of the DNAPL into saturated, heterogeneous porous media. They found that for the same amount of DNAPL released, higher DNAPL head resulted in smaller lateral spreading and higher average DNAPL saturation. Observations from one field experiment of PCE release in the vadose zone were in agreement with this finding (Poulsen and Kueper, 1992).

When selecting the DNAPL release conditions for the present study, high DNAPL head at the source is assumed to be preferable, mainly because of the following two concerns. The first is to avoid extensive lateral spreading, which can result in short-circuiting of PCE along the cell walls, as observed in both reported releases. Moreover, detection of PCE close to the sheet pile wall by ground penetrating radar is impossible, making the mass balance difficult and reducing the value of the data. The second concern is to increase the average residual saturation of the PCE, which may facilitate the detection of PCE by some geophysical methods.

2. Site Characterization Data Analysis and T2VOC Input Data Preparation

The numerical code T2VOC (Falta et al., 1995) requires the following soil-specific input parameters: soil permeability, porosity, and the capillary pressure-saturation and relative permeability-saturation constitutive relationships. As observed in the reported field releases, centimeter-scale variations in subsurface characteristics can significantly affect

DNAPL transport. The reviewed site characterization cone penetration test (CPT) data include soil classification number (SCN) and hydraulic conductivity estimated values. However, these data can provide only an order of magnitude estimation of localized hydraulic conductivity values or large-scale average values. Measurements of porosity and information on constitutive relationships are available only at a few locations. Direct soil sampling was not performed inside the test cell, due to the concern of protecting the integrity of the test cell.

Available grain-size distribution data were used to estimate the hydraulic conductivity and constitutive relationships based on empirical equations (Buesing and Pantazidou, 1996). Because the estimated values were not close to direct measurements, more powerful estimation methods were explored. The hydraulic conductivity and the variation of the soil type inside the test cell will also be estimated through kriging methods, using the programs from GSLIB (Deutcsh and Journel, 1992). Then the correlation between characteristic parameters and soil type at the measurement locations will be used to construct the input data for the test cell. Table 2 summarizes the sources and values of these parameters [Groundwater Remediation Field Laboratory (GRFL), 1995; 1996].

Table 2. Soil parameters from Dover site characterization data.

Input parameter	Source of data	Value
Hydraulic conductivity (cm/s)	Correlation with soil classification number (SCN) - CPT data	$10^{-1} - 10^{-6}$
	Grain size distribution (CPT-11)	$10^{-4} - 10^{-8}$
	Vadose zone IP[a] test (at 7 depths)	$1.28 \times 10^{-4} - 1.15 \times 10^{-3}$
	Pumping test and slug test	$K_z = (0.35 - 0.92) \times 10^{-3}$ $K_r = (0.76 - 11.7) \times 10^{-3}$
	Aquitard K from CPT data	$K_z = 1.4 \times 10^{-6}$ $K_r = 2.9 \times 10^{-6}$
Porosity	Vadose zone IP[a] test (at 5 depths)	$21\% - 32\%$
	Correlation with dielectric constant - CPT data (saturated zone)	$21\% - 25\%$
Capillary pressure curve (van-Genuchten model)	Vadose zone IP[a] test (at 5 depths)	$\alpha = 0.012 - 0.036 \, \text{cm}^{-1}$ $n = 1.7 - 3.5$

[a] IP = instantaneous profile test for hydraulic conductivity measurement in the vadose zone.

The CPT soil profiles indicate irregular occurrences of lenses of fine-grained soil at depths of 11 to 24 feet in the vicinity of the test cell. Through geostatistical analysis (variogram), the horizontal correlation length of soil classification number (SCN) at this depth range was estimated to be comparable to the test cell dimensions. Above and below this depth range, contrasts in soil type are less pronounced (clean sand to silty sand), with horizontal correlation lengths much higher than the size of test cell. Hence, the horizontal distributions of the SCN at the upper and lower sections are estimated to be relatively uniform across the test cell. Therefore, a 2-D axisymmetrical medium formation is expected to describe well the upper and lower sections, but be unable to represent the horizontal variation in the middle section of the test cell.

The uncertainty in soil type prediction can be reduced if cone penetration tests were conducted at locations closer to the test cell. Additionally, better estimation of the SCN distribution is possible through the correlation of ground penetrating radar data with the CPT data. However, such detailed data analysis is beyond the scope of this numerical modeling study.

3. Numerical Simulation

The possibility of using large-scale parameters to predict the major features of the DNAPL migration was tested with some preliminary simulations of the Borden field releases. An 8-hour segment of the PCE release in one of the Borden experiments (Kueper et al., 1995) was simulated using a 2-D homogeneous formation including a single low permeability layer. The site characterization data for the Borden aquifer have been extensively reported (Kueper and Frind, 1991; Poulsen and Kueper, 1992), providing good input for this simulation.

The modeling results of a simulated constant flux release are shown in Figure 1. The experimentally observed PCE pool above a horizontal low permeability layer is clearly reproduced in Figure 1. The pool is predicted to extend over 0.9 meter, rather close to the experimental measurement of 1.1 m. This result supports the assumption that numerical models can predict the major features of the DNAPL plume as long as the model domain accounts for the large-scale geologic features. On the contrary, the constant head simulation gave a release rate higher than the experimental observation. This may partly be explained by the hypothesis proposed by Kueper and Gerhard (1995), namely that the release rate depends primarily on the permeability of the soil near the source. The release rates of the Borden experiments differ from each other, despite the fact that the release conditions are very similar, the test cells are only 10 meters apart and the aquifer is relatively homogeneous.
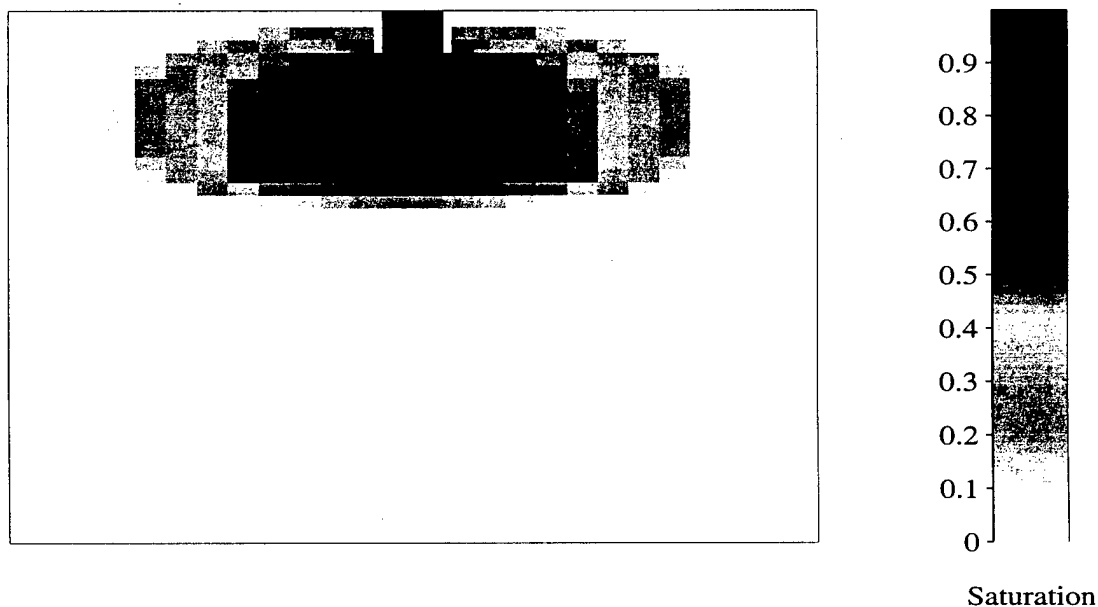

Saturation

Figure 1. Simulation of PCE release at Borden site, after 8-hour constant flux injection.

Various simulation domains will be evaluated for the Dover test cell, including a 2-D homogeneous medium, a 2-D layered medium and a 3-D heterogeneous medium, to investigate the effect of vertical and horizontal heterogeneity. For each realization, different DNAPL heads will be considered. These simulations are currently being conducted.

Future sensitivity analysis may include using the GSLIB programs to generate multiple medium formations in order to observe the effect of input data uncertainty on the transport patterns. The influence of relative scale of DNAPL head, correlation scale of heterogeneity, size of test cell and contrasts in soil properties on the simulation results may also be evaluated.

Acknowledgment/Disclaimer

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